Model 1: Simulation of hydrogen production system

Simulating the distribution of hydrogen and oxygen among our system has essential implications for further experiments.

1. Single-bacteria model

We assume that every *E.coli* cell is a source that releases hydrogen. The concentration of hydrogen exponentially decreases by distance. It is easily known that microballs are spherically symmetric. The following figure shows the distribution of hydrogen in this model:

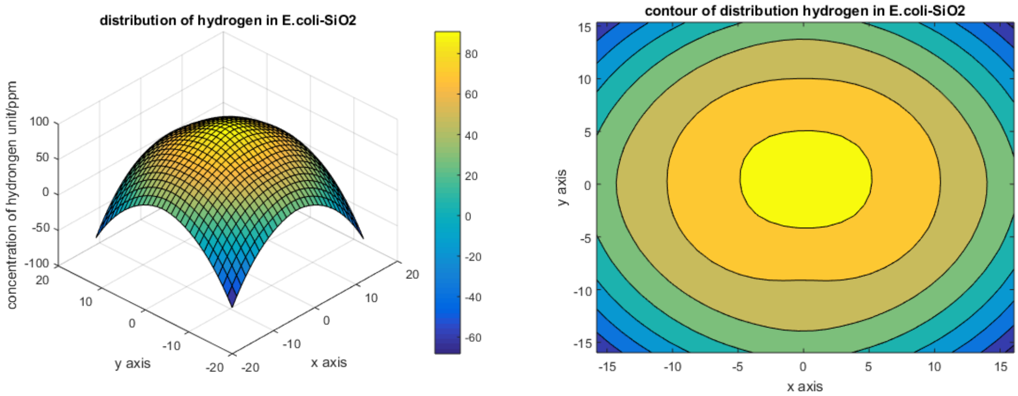

Figure 1 hydrogen distribution in *E.coli*-SiO2 microballs

2. Multi-bacteria model

Consider a more complex condition where a nesting system is built by multi-layered polymer coats and *E.coli* cells during encapsulation. Every hydrogen source interacts with each other. We employ the formulations of gas diffusion dynamics considering the 50µm scale of microballs.

The followings are our assumptions:

(i) A stratified spherical structure is constructed by polymers and *E.coli* cells along with CdS particles. This shapes like a plum-pudding sphere.

(ii) Abundant cells are averagely distributed within the system. As this system is spherically symmetric, we will only consider the concentration gradient on a single radius.

(iii) There exist a threshold for hydrogen production of the bacteria: only when oxygen level drops to a certain degree will *E.coli* cells produce hydrogen.

(iv) All gases undergo passive transport through the channels in the system.

The differential equations is on the basis of the diffusion equation with source term because the convention term can be neglected in such small region. Only when oxygen concentration is under the threshold can cells release hydrogen. Meanwhile the cells will consume the oxygen until the concentration of oxygen drops to zero.

To include all these interactions into our model, we are now adding cross terms into hydrogen-oxygen equations:

$$
\begin{cases}
0 = -D_H(r)\nabla^2 c_H(r) + g(r) q_H(c_O) \\
0 = -D_O(r)\nabla^2 c_O(r) + g(r) q_O(c_O) \\
c_H(r_0) = 0 \\
c_O(r_0) = c_{O,inital} \\
c_H{}'(r_0) = 0 \\
c_O{}'(r_0) = 0
\end{cases}
$$

$$
q_H(c_O) = \begin{cases} 1, c_O < c_{O,critical} \\ 0, otherwise \end{cases}
$$

$$
q_O(c_O) = -\left(1 - e^{-s \cdot c_O}\right)
$$

$$
g(r) = \begin{cases} \sin kr, \sin kr > 0 \\ 0, otherwise \end{cases}
$$

$$
D_{O,H}(r) = g(r) = \begin{cases} \sin(kr+\pi), \sin(kr+\pi) > D_{0,O,H} \\ D_{0,O,H}, otherwise \end{cases}
$$

In equations:

D_H And D_O are the diffusion coefficient for hydrogen and oxygen. c_O and c_H are the concentration. r_0 is the radius of the total bacteria ball. q_H and q_O are the source intensity for hydrogen and oxygen. s is the sensitive coefficient.

Considering the stratified structure of the bacteria microballs, we introduce a geometry function to describe it, namely $g(r)$.

The boundary condition is the concentration of the oxygen and hydrogen, it depends on the experiment, and the gradient of them is zero for hydrogen is passive transport. A stable solution for hydrogen and oxygen concentration according to the differential equations above shows below in which the blue curve represents hydrogen while yellow represents oxygen (Figure 2).

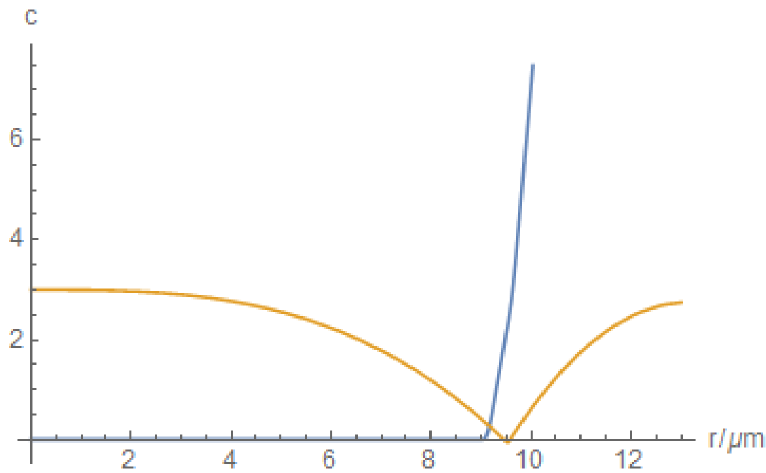

Figure 2 stable solution for hydrogen and oxygen according to differential equations

Then when we randomly change the concentration of exterior oxygen, we found homeostasis solution for hydrogen (Figure 3left) and oxygen (Figure 3right). The curves develop in a similar trend.

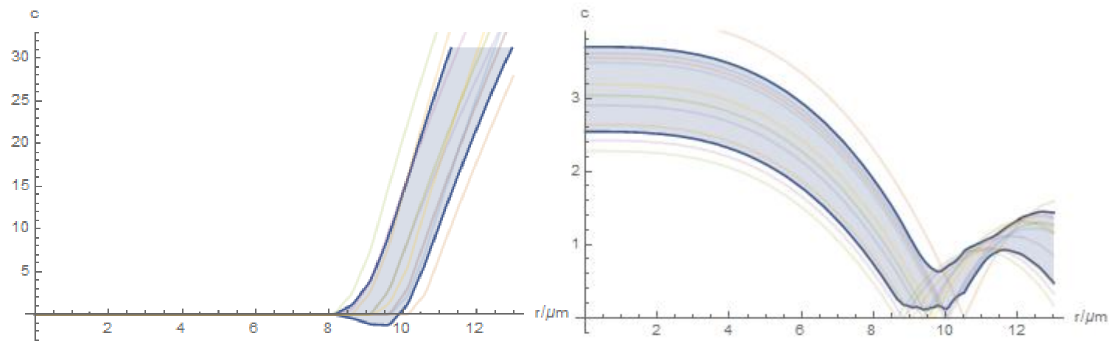

Figure 3 homeostasis solution for hydrogen (left) and oxygen (right)